NETL Multiphase Flow Research Overview

NATIONAL ENERGY TECHNOLOGY LABORATORY

NETL Workshop on Multiphase Flow Science

8/3/2021

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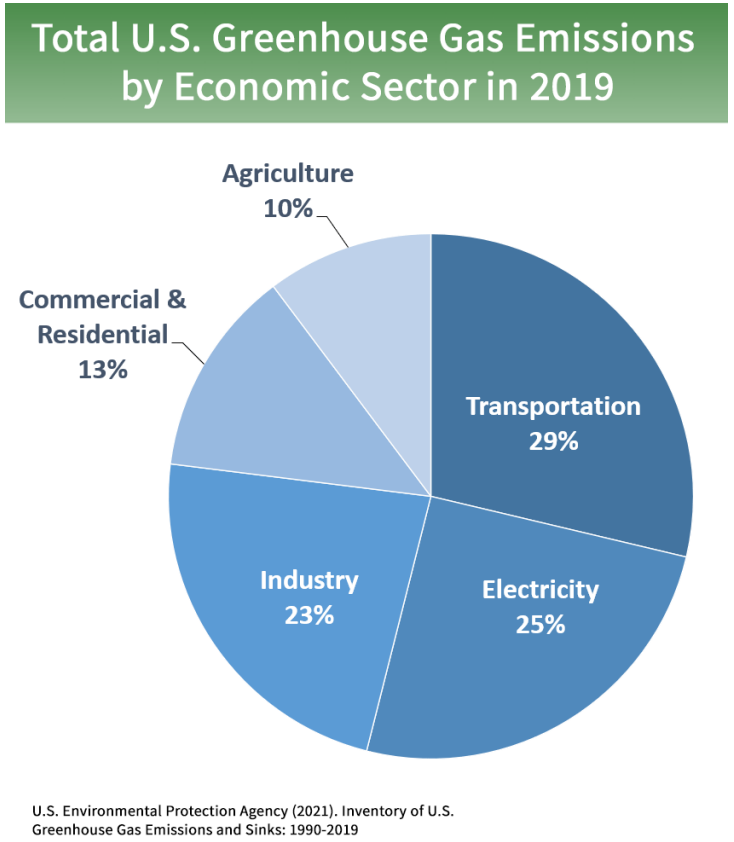
Senior Fellow for Computational Science & Engineering

"Our New Name is also a New Vision"[1]

- President Biden's goals:
  - CO_2 emissions--free power sector by 2035
  - Net zero emissions economy by no later than 2050
- DOE-FE is now DOE-FECM – Office of Fossil Energy **and Carbon Management**
  - Point source carbon capture
  - CO_2 removal
  - CO_2 conversion into products
  - Reliable CO_2 storage
  - Blue hydrogen production
  - Critical minerals production



1. Wilcox J, Talati S. Our New Name is also a New Vision. July 2021. https://www.energy.gov/fe/articles/our-new-name-also-new-vision

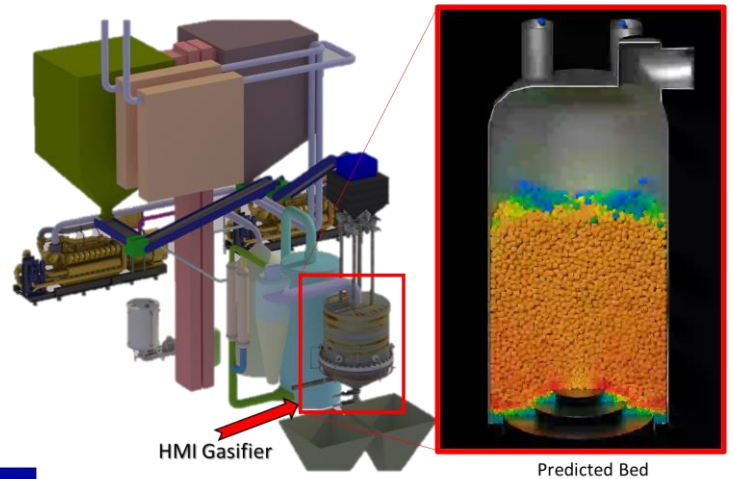
Recent MFIX applications at NETL relevant to carbon management

Supporting the design of a 22 MW_{th} gasifier for a $46 M facility at University of Alaska-Fairbanks

- Predicted the performance of the **scaled-up gasifier** design for a range of operating conditions
- Evaluated novel operating conditions for reducing carbon emissions by simulating
  - Oxygen-blown operation
  - Coal-biomass co-feed

Simulation-based engineering for bioenergy applications

- Development and troubleshooting of NREL **entrained flow pyrolysis reactor** for H_2-enriched operations.
- Troubleshooting capacity problems with **catalytic vapor-phase upgrading unit** for NREL pilot-scale catalytic fast pyrolysis unit.

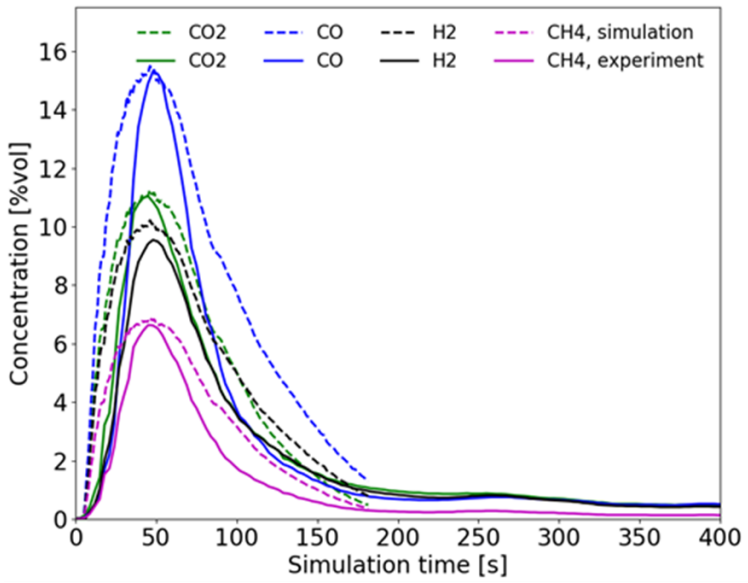


UNIVERSITY OF ALASKA FAIRBANKS · HMI · SOTACARBO SUSTAINABLE ENERGY RESEARCH CENTRE · PARSONS

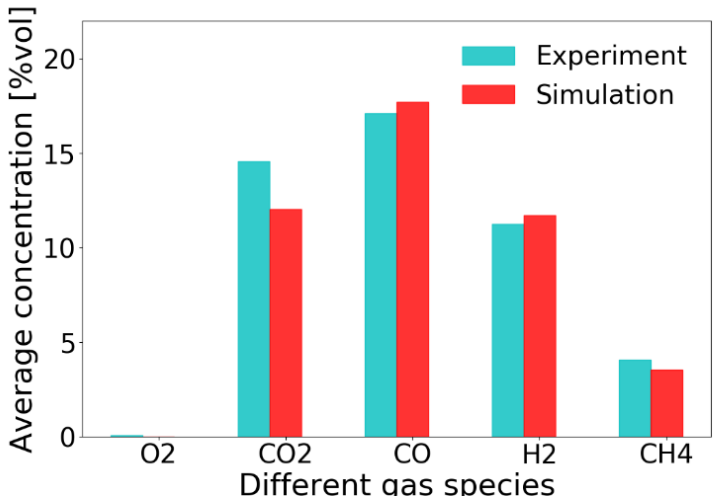
The ORNL-NETL-NREL team designed and installed an additional cyclone that enabled a 10 kg/hr biomass feed rate with full catalyst regeneration

This ~$100k modeling effort enabled the $1.9M/year project to meet a key milestone

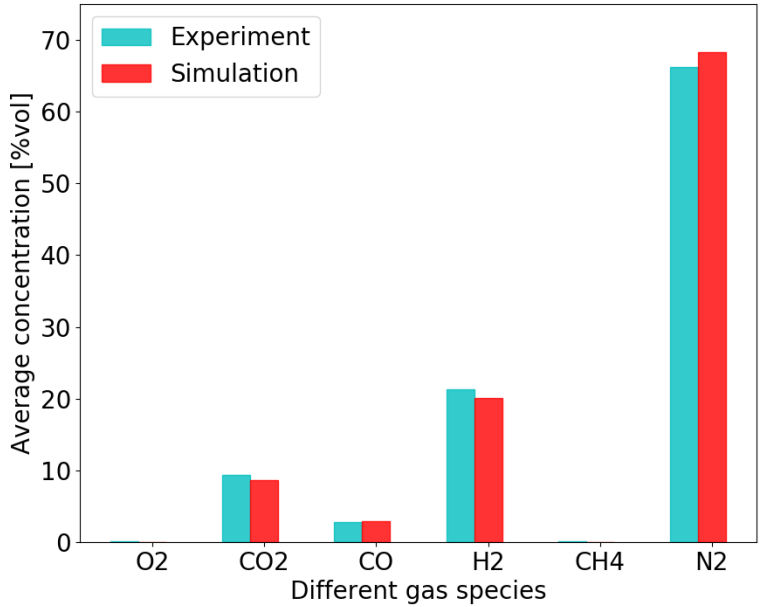
Biomass gasifier modeling in collaboration with Sotocarbo



Pyrolysis



Biomass Combustion & Gasification



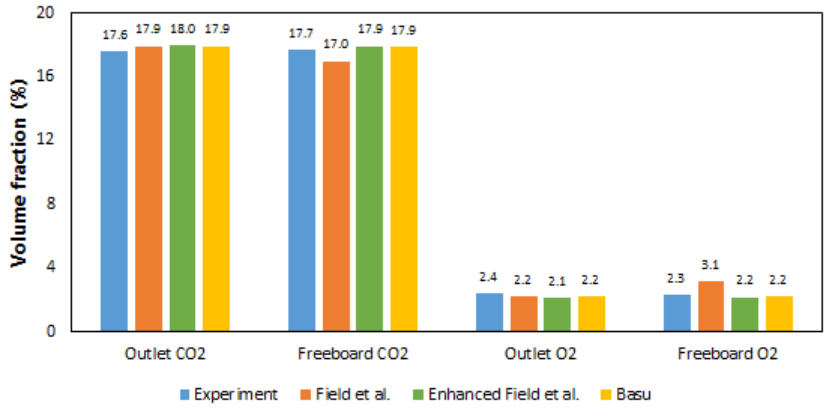
Char Gasification

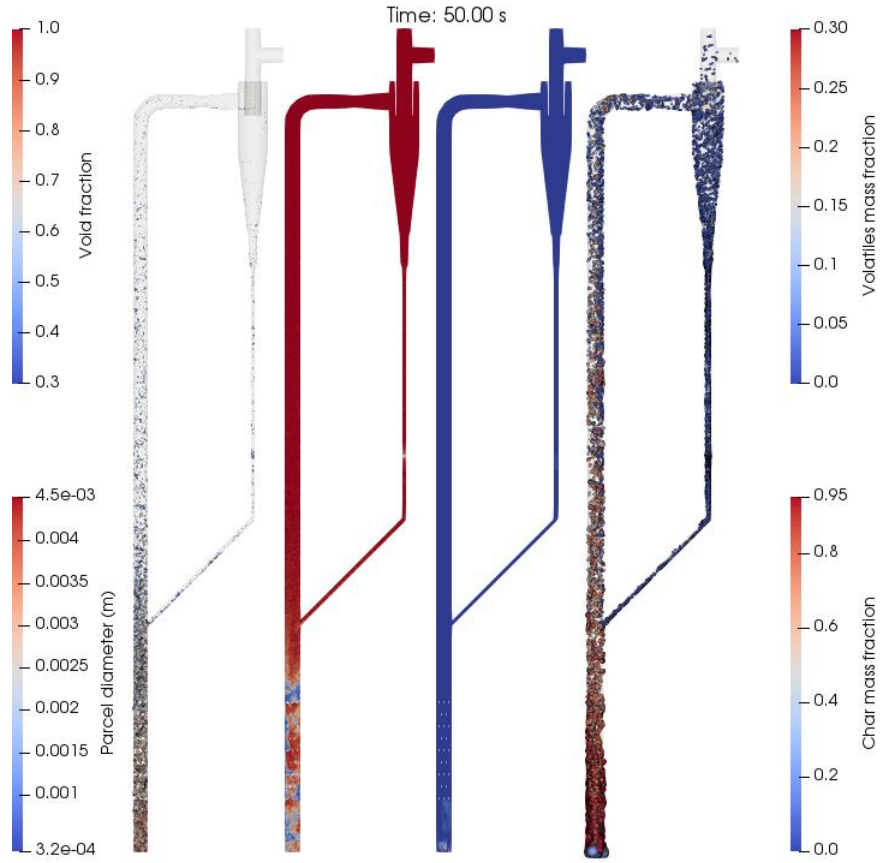
SOTACARBO
SUSTAINABLE ENERGY RESEARCH CENTRE

Porcu A, Xu Y, Mureddu M, Dessì M, Shahnam M, Rogers WA, Sastri BS, Pettinau A. Experimental validation of a multiphase flow model of a lab-scale fluidized-bed gasification unit. *Applied Energy* 293 (2021): 116933.

Biomass combustor modeling in collaboration with CanmetENERGY

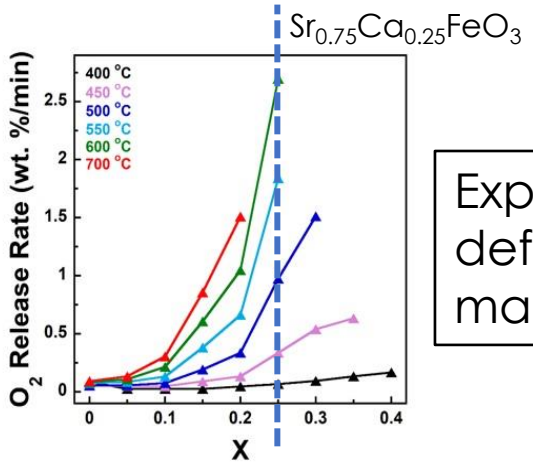
- Developed an MFIX-PIC model of 50kW$_{th}$ circulating fluidized bed combustor at CanmetENERGY, Natural Resources Canada
- The combustion model was validated with CanmetENERGY data.
- The model can be readily adapted for a variety of biomass fuels as well as co-fired systems under air and oxy-fuel conditions



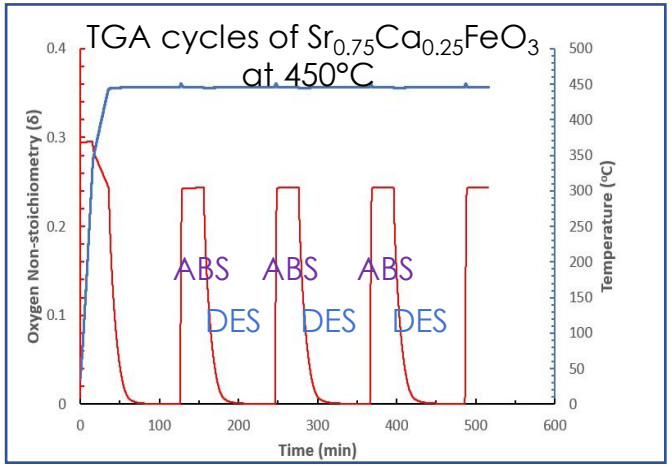


1. Banerjee S, Hughes RW. Biomass Combustion in a Circulating Fluidized Bed Combustor; DOE/NETL-2020/2148; DOI: 10.2172/1659115.
2. Banerjee S. Full-Loop Simulation of the Combustion of Biomass in a Circulating Fluidized Bed Combustor; DOE/NETL-2021/2650. DOI: 10.2172/1785675.

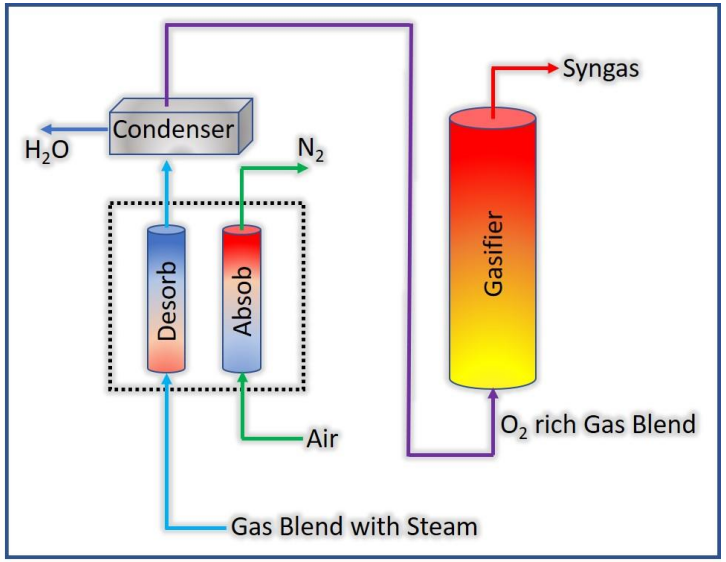
Perovskite sorbent oxygen separation modeling

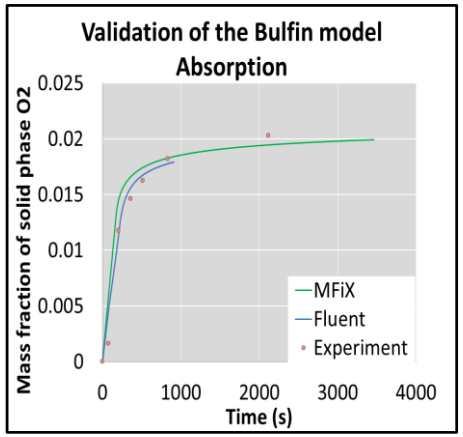


Experimentalists define best material



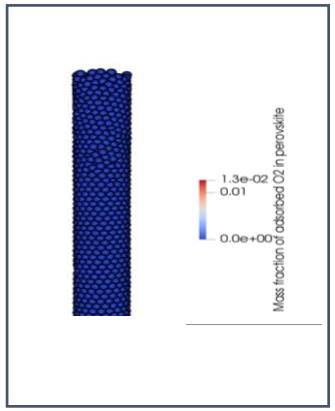
$$Sr_{0.75}Ca_{0.25}FeO_3 \xleftrightarrow{\delta(T,P_{O_2})} Sr_{0.75}Ca_{0.25}FeO_{3-\delta} + \frac{\delta}{2}O_2$$





Micro-scale simulation validates kinetic rates

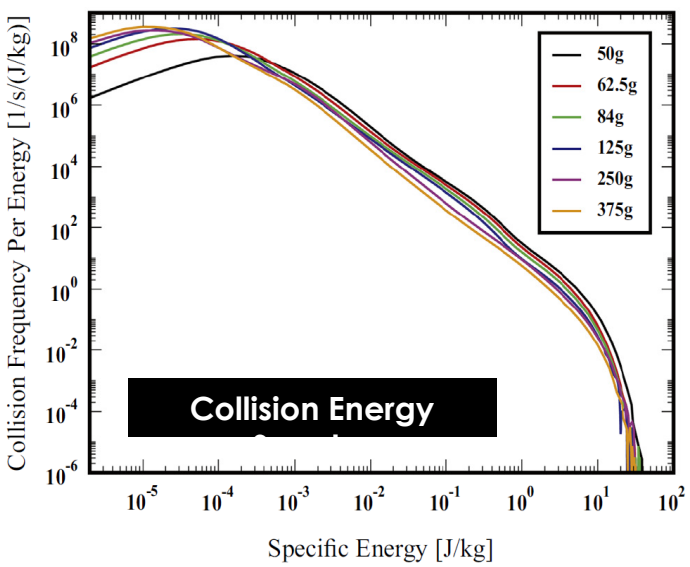
Small-scale simulation extends understanding

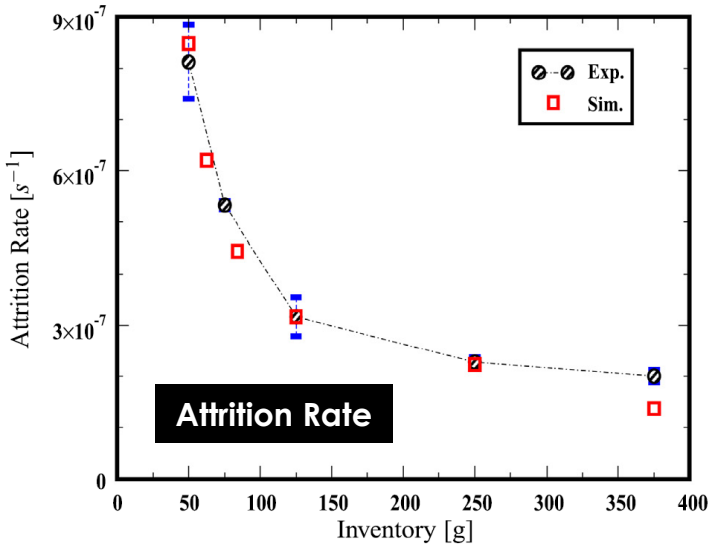


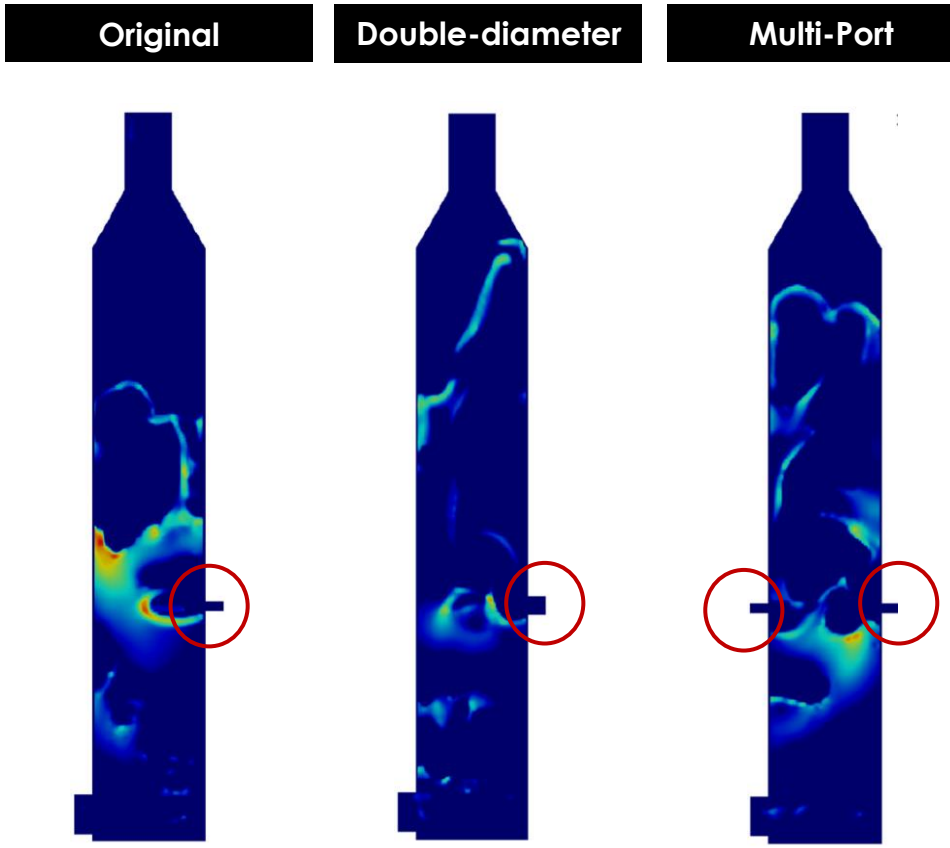
Process model extends to larger-scale simulation

Chandramouli D, Clarke M. Perovskite sorbent oxygen separation modeling with MFiX. NETL Technical Report Series; U.S. Department of Energy, National Technology Laboratory: Morgantown, WV, 2021.

Chemical looping reactor redesigned for reducing attrition rate







Instantaneous local attrition rate

(Dark Blue: $8x10^{-13}s^{-1}$, Dark Red: $8x10^{-10}s^{-1}$)

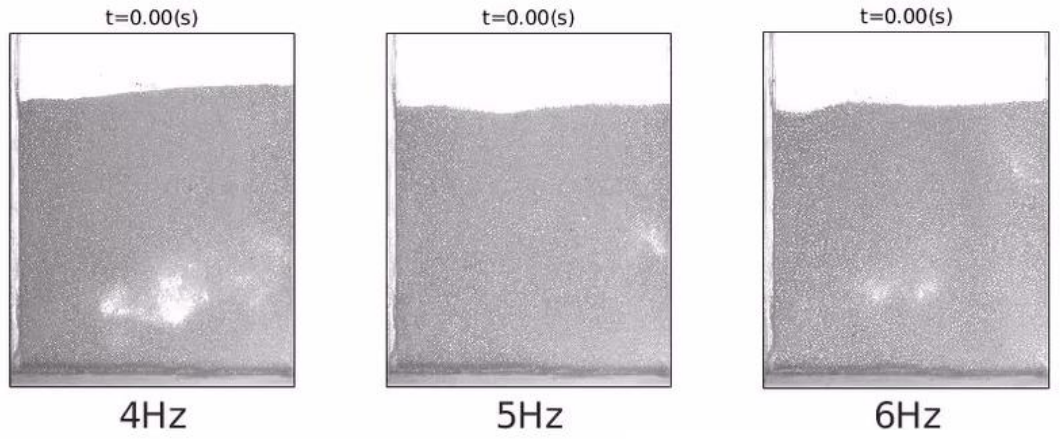
- Attrition model, based on a computed energy spectrum, was validated with Jet Cup data[1]
- Analyzed 2 proposed Air Reactor designs; "Double-diameter" design reduces the attrition rate by 34% [2]

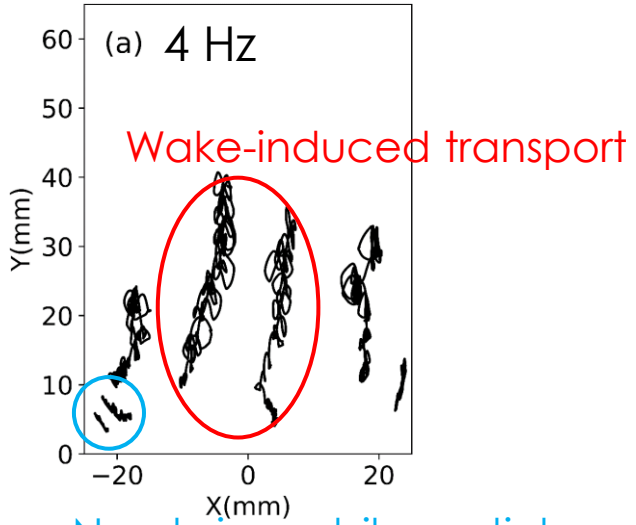
1. Konan NA, Huckaby ED. *Powder Tech.* *(2021)* https://doi.org/10.1016/j.powtec.2021.06.014
2. Konan NA, Huckaby ED. *Powder Tech.* *(2021)* https://doi.org/10.1016/j.powtec.2021.06.010

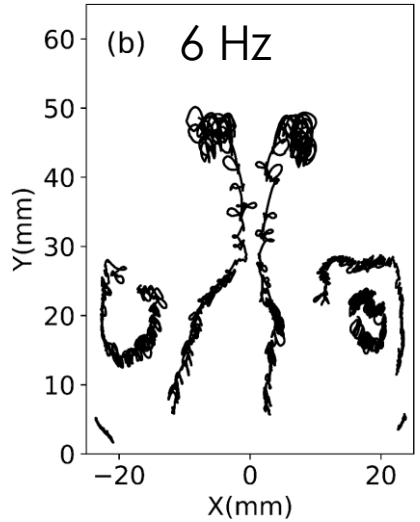
Meso- and micro-scale analysis of a pulsed fluidized bed

- Meso-scale: bubbling pattern and collective solids motion
- Micro-scale: individual particle motion
  - Space-time varying anomalous diffusion
  - Long-range processes characterizing system's memory identified through auto-correlation
- Found at both the scales
  - Harmonic and sub-harmonic responses to pulsing
  - Suppression of chaos at higher frequencies

Bench-scale pulsed fluidized bed experiments at NETL



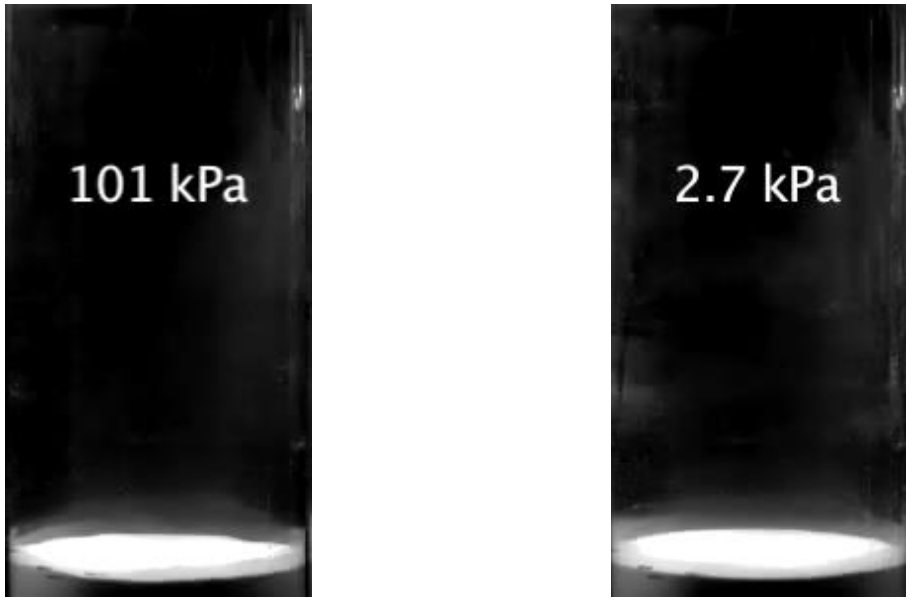




1. Higham JE, Shahnam M, Vaidheeswaran A. (2020). Using a proper orthogonal decomposition to elucidate features in granular flows. *Granular Matter*, 22(4), 1-13.
2. Higham JE, Shahnam M, Vaidheeswaran A. (2021). Anomalous diffusion in a bench-scale pulsed fluidized bed. *Physical Review E*, *103*(4), 043103.

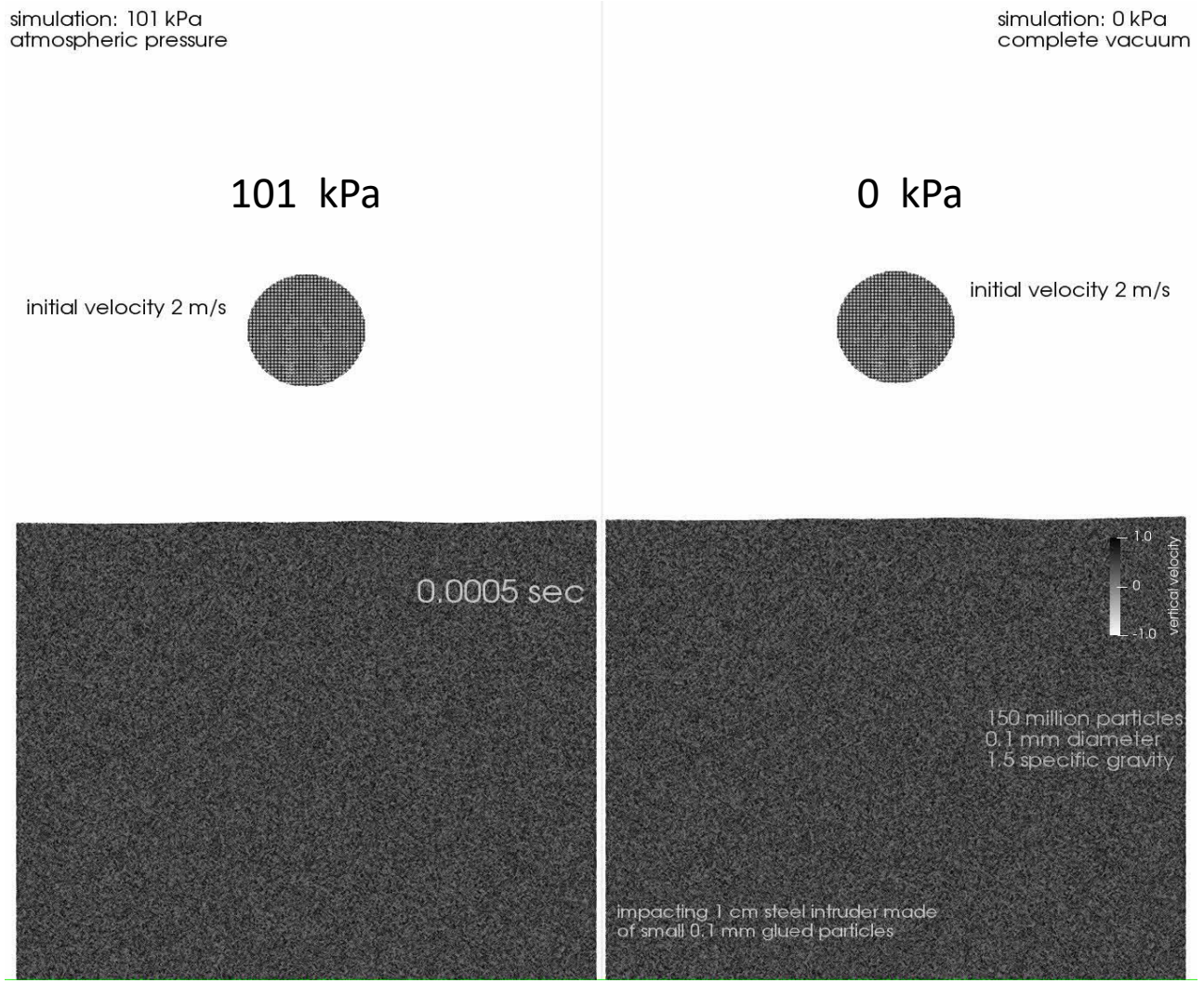
CFD-DEM simulation of granular jets under two pressure conditions

Experiment



Courtesy: H. Jaeger, U. of Chicago

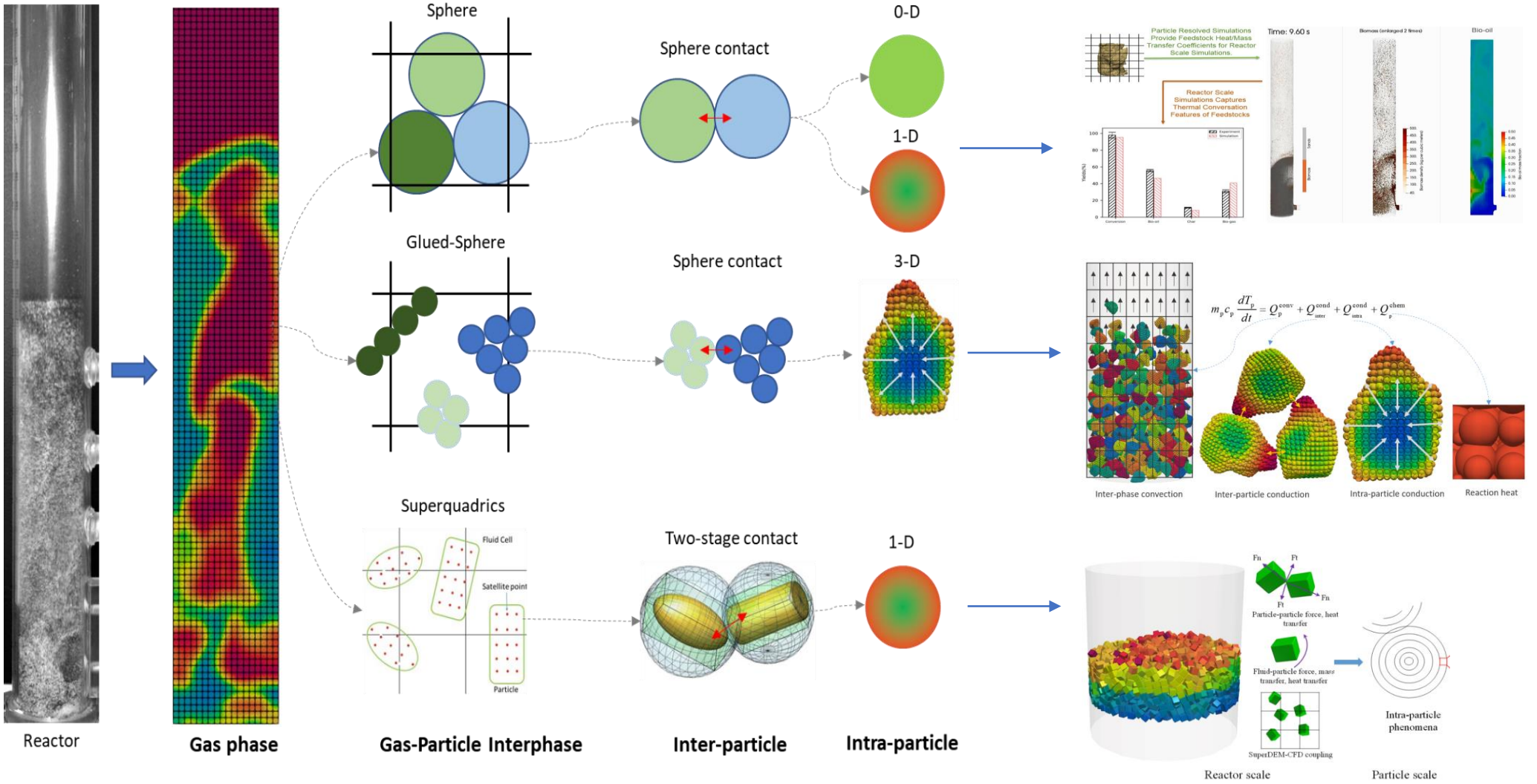
Simulation



More than 150 M particles and 3.5 M fluid cells simulated on Joule 2 supercomputer.

Benyahia S. *Ind. Eng. Chem. Res*. 2020, 59, 8416−8425.
doi: 10.1021/acs.iecr.0c00808

Multi-Scale shape-resolved CFD-DEM simulations of biomass fast pyrolysis



[Lu et al., 2020, Chem. Eng. Sci. https://doi.org/10.1016/j.ces.2020.115471](https://doi.org/10.1016/j.ces.2020.115471)

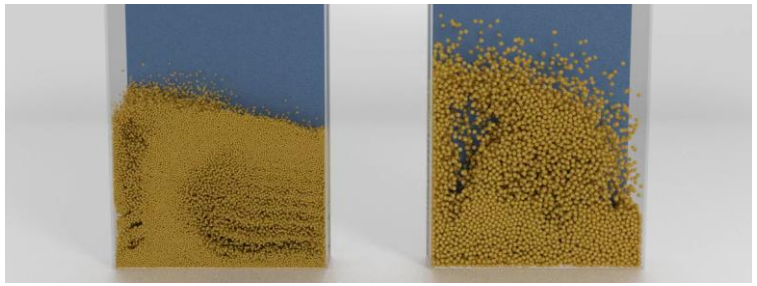
[Lu et al., 2021, Chem. Eng. J. https://doi.org/10.1016/j.cej.2021.129564](https://doi.org/10.1016/j.cej.2021.129564)

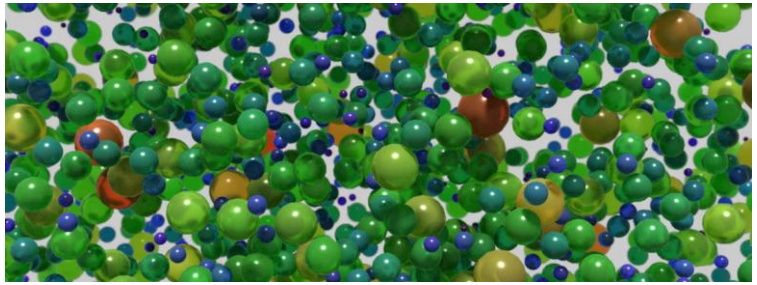
[Xi et al., 2021, AIChE J. https://doi.org/10.1002/aic.17139](https://doi.org/10.1002/aic.17139)

MFiX development

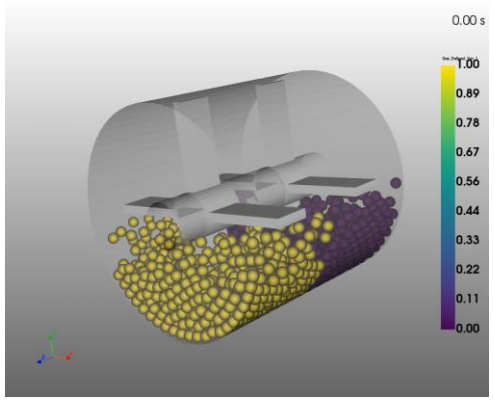
- Recent released capabilities
  - 21.1: 2x faster flow solver
  - 20.4: Coarse Grain DEM
  - 20.3: DEM Polydispersity
  - 20.2: Moving geometry for granular flows
  - 20.1: New meshing workflow
- Current developments
  - Non-spherical particles (glued sphere, Superquadrics)
  - GPU porting of DEM (80x speedup)
  - DEM Rolling friction
  - PIC parameter sensitivity/calibration
- Outreach
  - All-time MFiX registrations ≈ **7,000**
  - Registrations:+24%, Downloads:+75%

DEM vs Coarse Grain DEM

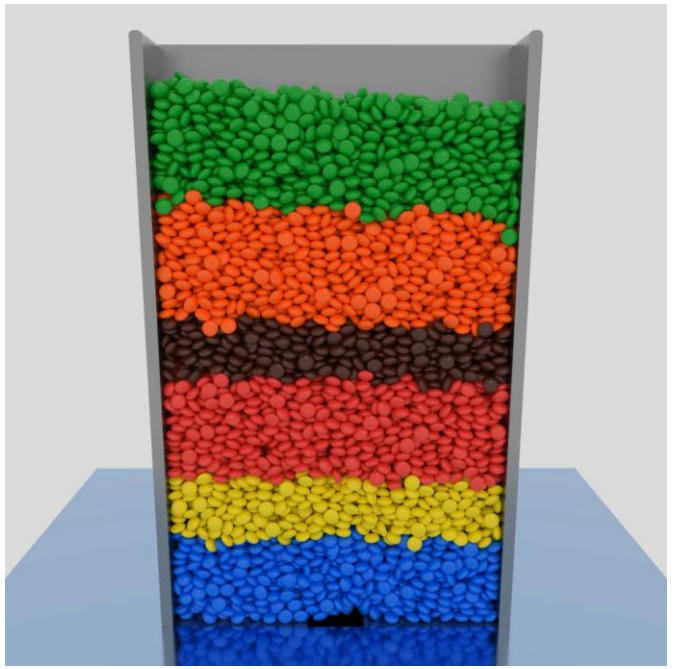




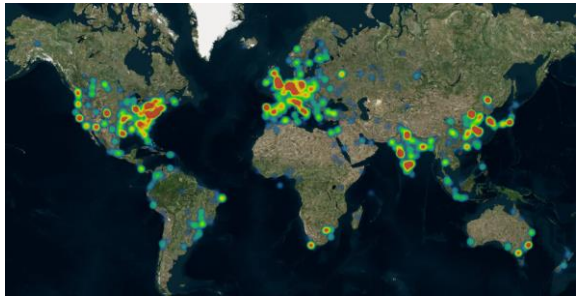
Polydispersity



Moving geometry

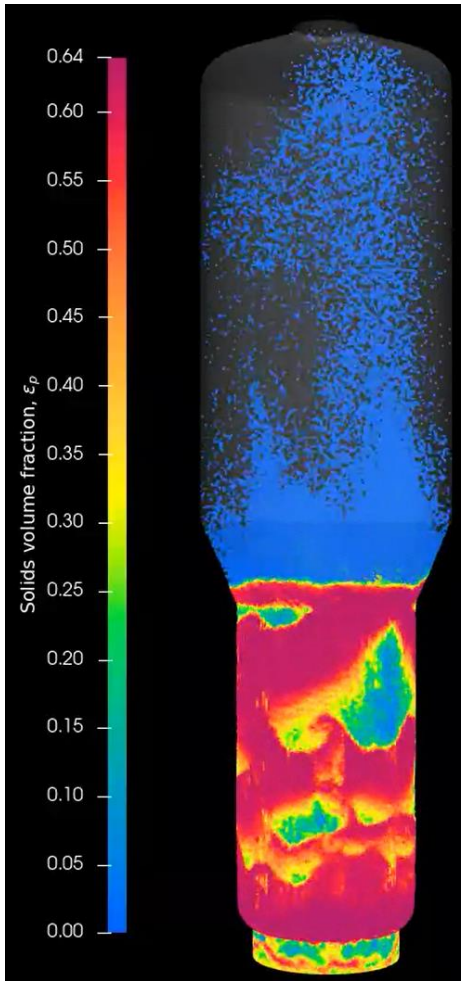


Superquadrics



MFIX registrations in 2020

MFIX-Exa: a path towards Exascale CFD-DEM simulations



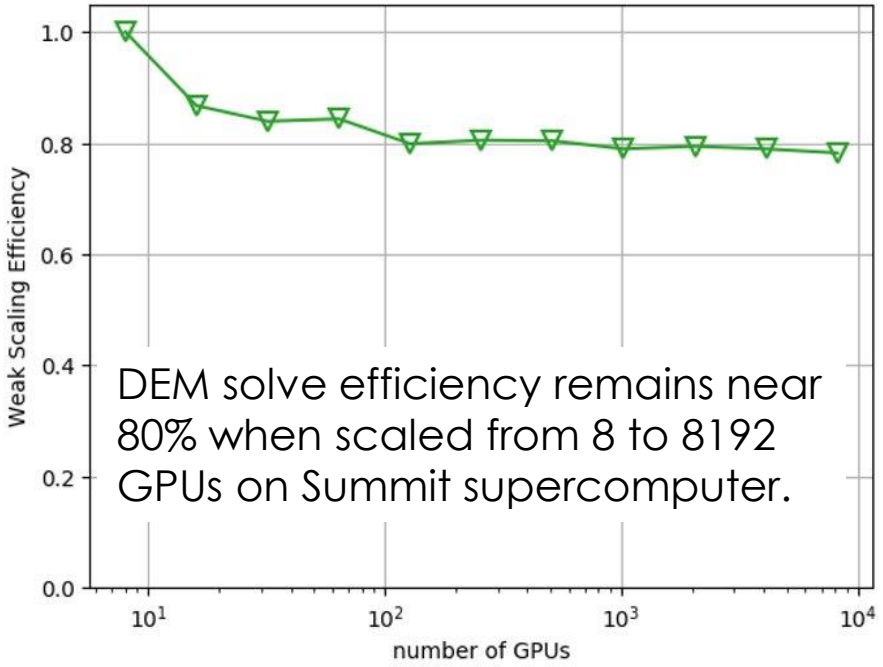
MFIX-Exa PIC simulation

Recent development advancements

- 2nd Order Godunov advection scheme
- CSG based geometry interpreter
- GPU based particle-in-cell model

Preparing for Exascale machines

- **Oak Ridge development system:**
  Spock: *AMD EPYC CPU / 4x AMD MI100 GPUs.*
- **Argonne development system:**
  Arcticus: *Intel XeHP using oneAPI Toolkits*



Musser J, Almgren AS, Fullmer WD, Antepara O, Bell JB, Blaschke J, Gott JK, Myers A, Porcu AR, Rangarajan D, Rosso M, Zhang W, Syamlal M. MFIX-Exa: A Path Towards Exascale CFD-DEM Simulations. *The International Journal of High Performance Computing Applications*. 2021. doi:10.1177/10943420211009293

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0.86 Petaflop/s achieved on a CS-1 for the BiCGStab linear equation solver

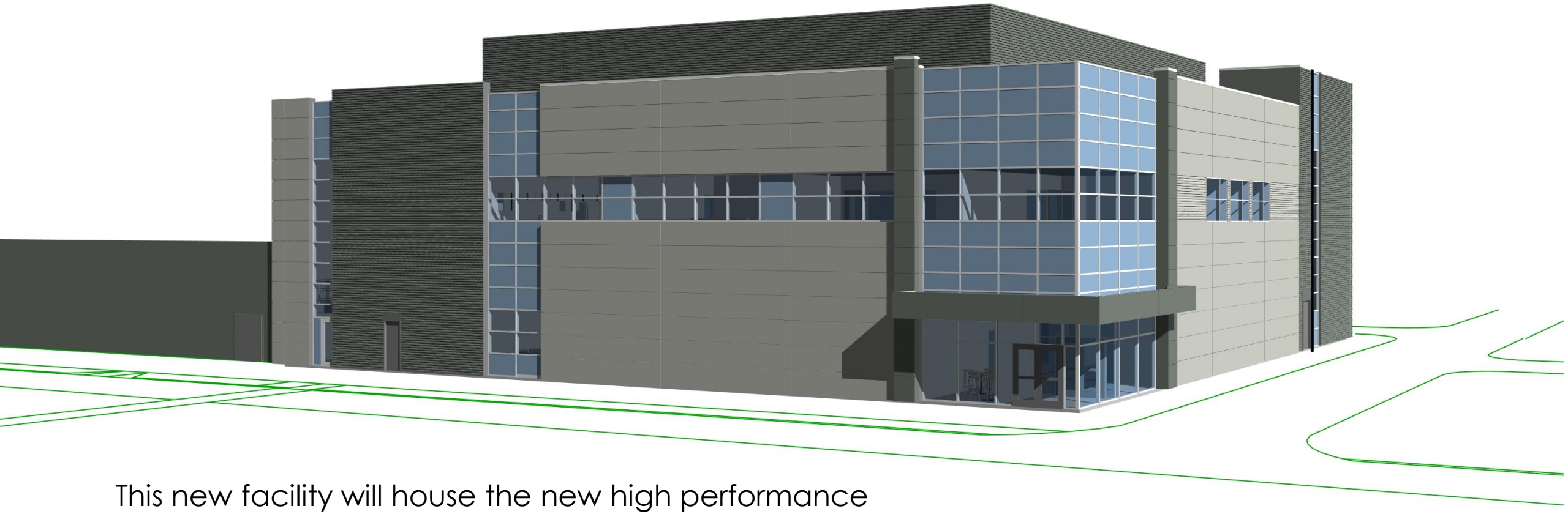
A Wafer-Scale Engine, "the world's largest chip," powers the deep learning system **Cerebras CS-1**

370x370x370 ≈ 51 M cells	Joule 2.0 (double precision)	CS-1 (mixed precision)
Wall time/iteration (µs)	2100	6
Achieved speed (Tflop/s)	1.1	371
% of theoretical max speed	0.35	30
600x595x1536 ≈ 548 M cells		
Wall time/iteration (µs)		28
Achieved speed (Tflop/s)		860
% of theoretical max speed		30

Rocki K, Van Essendelft D, Sharapov I, Schreiber R, Morrison M, Kibardin V, Portnoy A, Dietiker JF, Syamlal M, James M. Fast Stencil-Code Computation on a Wafer-Scale Processor. arXiv:2010.03660v1 [cs.DC] 7 Oct 2020

Computational Science and Engineering Center Building

Completion expected around October 2023



This new facility will house the new high performance computing center, visualization room and provide space for approximately 50 research personnel.

NETL, MORGANTOWN, WV

Thanks, Multiphase Flow Researchers at NETL!

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